

# Quantum Evolution Supergenerator of Superparamagnetic System in Discrete Orientation Model

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## Abstract

The supergenerator of superparamagnetic system quantum evolution is investigated in discrete orientation model (DOM). It is shown that the generator is  $J$ -self-adjoint one at the case of potential drift field agreed upon magnetic anisotropy of the sample investigated. Perturbation theory is used for spectral analysis. The qualitative dependence of resonance absorption spectrum on the relation between quantum and stochastic parameters is demonstrated.

keywords: superoperator, superparamagnetic, Mössbauer spectroscopy

## Introduction

Qualitative and quantitative description of relaxation Mössbauer spectra is based on choosing of some relaxation process model. In the most general model of motion of magnetic moment  $\vec{M}(t)$  suggested by Brown [1] this motion is considered like diffusion process on radius  $|\vec{M}|$  sphere in a drift field stipulated by the magnetic anisotropy of the pattern. Under Born's approximation Mössbauer spectra line shape one can express in terms of resolvent of the generator of quantum evolution operator of a nucleus, averaged along all diffusion process  $\vec{M}(t)$  trajectories. But computation of averaged evolution operator is connected with solving of complicated differential equation system of partial derivatives and can not be done in analytical form. To avoid this difficulty phenomenological models are used, where magnetic moment  $\vec{M}(t)$

position becomes discrete, and process of  $\vec{M}(t)$  motion itself is replaced by Markovian process with final number of states, which is described by stochastic matrix with phenomenological transition probabilities of the magnetic moment  $\vec{M}(t)$  from one state (of easy magnetization) to another (so called discrete orientation model (DOM)). In this case the problem of computation of averaged evolution operator obtains algebraic character and reduces to inversion of special matrices, which properties and order are determined by the number of easy magnetization directions, the structure of nucleus magnet electron system and by the symmetry of pattern. In this direction certain progress was reached for SP particles with cubic symmetry [2]. Direct account of symmetry in frames of phenomenological DOM permitted authors [2] to reduce the calculation of absorption line shape of SP particles to inversion some matrices of 8- and 6- order for cubic symmetry systems with negative and positive magnetic anisotropy constants respectively.

For the case of large values of reduced barrier  $\alpha = KV/kT$ , where  $K$  is magnetic anisotropy constant,  $k$  - Boltzmann constant,  $V$  - volume of SP particle,  $T$  - temperature, DOM parameters one can calculate by the lowest eigenvalues of Fokker-Plank equation [3], [4], giving evolution of  $\vec{M}(t)$  in diffusion model [5], and line shape calculated in such a way is the leading term under  $\alpha \rightarrow \infty$  of line shape calculated on the base of diffusion model [6]. For accurate calculation of the line shape error under substitution of diffusion model to discrete one (DOM) first of all detailed analysis of the generator of averaged evolution operator of a nucleus in frames of DOM is necessary.

In present paper, developing symmetry considerations stated at [2], we investigate the structure of complete averaged evolution operator corresponding to DOM for cubic symmetry (with 6 and 8 easy magnetization directions on  $Fe^{57}$  nucleus) and some others, maintain it's spectral analysis in frames of perturbation theory under assumption of slow relaxation and also describe qualitative picture of spectrum behavior in general case (subject to temperature). In proper basis the generator matrix is composed of equal blocks of  $8 \times 8$  order differing only by its diagonal elements composed by combinations of eigenvalues of the stochastic matrix giving DOM. Non-diagonal part of such block is determined only by the nuclear system structure and does not depend neither on stochastic variables nor on crystal lattice symmetry type (on magnetic anisotropy constant sign for cubic symmetry).

# 1 Basic Formulas

In DOM magnetic moment evolution is defined by matrix  $P = S^T - I$ , where  $S$  is stochastic matrix of transition probabilities between easy magnetization states in unit of time. Vector  $\vec{g}(t)$  of magnetic moment  $\vec{M}(t)$  distribution is governed by ordinary differential equation

$$\frac{d\vec{g}}{dt} = P\vec{g}, \quad \vec{g} = (g_1, g_2, \dots, g_N)^\dagger, \quad (1)$$

where  $N$  - the number of process states (easy magnetization directions). In the case of cubic symmetry  $N$  is equal either 6 or 8 for positive or negative magnetic anisotropy constant respectively. Matrix  $P$  is naturally to call as Markovian one.

Line shape is determined by expression [2],[7]

$$\varphi(\omega) = \frac{2}{\Gamma} \text{Re} \int_0^\infty e^{(i\omega - \Gamma/2)t} Sp(\mathbf{V}^* \overline{G(t)} \mathbf{V} \rho) dt, \quad (2)$$

where  $\omega$  is the electromagnetic frequency,  $\Gamma$  - natural half-width,  $\rho$  - the initial state density matrix,  $\mathbf{V}$  - the operator of interaction of the nucleus with electromagnetic field,  $\overline{G(t)}$  - the result of averaging of the quantum evolution superoperator of the nucleus  $\exp(i \int_0^t \hat{L} d\tau)$  along all diffusion process trajectories, in our case along trajectories of Markovian process (1) with finite number of states. In this connection  $\overline{G(t)}$  is the solution of equation [7]:

$$\frac{d\overline{G}}{dt} = \hat{P}\overline{G} - i\hat{L}\overline{G}. \quad (3)$$

Here  $\hat{L}$  is diagonal on stochastic variables Liouville's superoperator, which action on the spin transition operators  $B$  is determined by the rule:  $\hat{L}B = H^e B - B H^g$ . Here  $H^{e,g} = A^{e,g} \times (\vec{I}^{e,g}, \vec{m})$ ,  $\vec{I}$  spin operator of a particle (for  $Fe^{57}$ :  $I^g = \frac{1}{2}$ ,  $I^e = \frac{3}{2}$ ),  $\vec{m}$  - unit vector of particle magnetization direction,  $A^{e,g}$  - hyperfine interaction constants,  $\hat{P} = P \otimes E_q$  - operator matrix diagonal on nuclear variables,  $E_q$  - identity superoperator acting in quantum states space.

Calculating integral (2) taking into account (3) one can get the following expression for line shape [2]

$$\varphi(\omega) = Im \sum_{a,b}^N \rho_a \langle \vec{\eta}^* J(a | \hat{L} + i\hat{P} - \lambda \hat{E} |^{-1} b) \vec{\eta} J^\dagger \rangle, \quad (4)$$

where  $\lambda = \omega + i\frac{\Gamma}{2}$ ,  $\Gamma$  - natural half-width,  $\vec{\eta}$  - vector of polarization of falling  $\gamma$ -radiation,  $J$  - nuclear current operator, responsible for transitions between sublevels of ground  $|m_g\rangle$  and excited  $|m_e\rangle$  nucleus states,  $\rho_a$  - relative probabilities of population of electron states  $a$  (there are  $N$  such states). So such calculation is reduced to spectral analysis of the generator of quantum evolution superoperator of a nucleus  $\hat{G}^{-1}(\lambda) = \hat{L} + i\hat{P} - \lambda\hat{E}$ , acting in space of operator-functions of the form:  $|\Psi\rangle = |m_e\rangle\langle m_g || a\rangle$ , which is a tensor product of the spin operators space and stochastic space of magnetic moment directions. Superoperator  $\hat{L}$ , responsible for hyperfine decomposition of levels, acts by the rule

$$\langle \Psi | \hat{L} | \Psi' \rangle = [H_{m_e m'_e}^e \delta_{m_g m'_g} - H_{m'_g m_g}^g \delta_{m_e m'_e}] \delta_{aa'}. \quad (5)$$

Operator matrix  $\hat{P}$  is diagonal on nuclei variables

$$\langle \Psi | \hat{P} | \Psi' \rangle = p_{aa'} \delta_{m_e m'_e} \delta_{m'_g m_g}, \quad (6)$$

$$p_{aa} = - \sum_{a' \neq a} (a | \hat{P} | a').$$

Relaxation matrix elements  $p_{aa'}$  are transition probabilities in unit of time from state  $a$  to state  $a'$ .

Of course one can consider the state  $|\Psi\rangle$  at (5) and (6) as usual state in direct product space of variables  $m_e$ ,  $m_g$ ,  $a$  and forget the superoperator nature of  $\hat{G} = (\hat{L} + i\hat{P} - \lambda\hat{E})^{-1}$ .

## 2 Spectral Analysis of Stochastic Matrices

Let us suppose that easy magnetization axes coincide with axes of 3(4)-order of cube for the case of negative (positive) magnetic anisotropy constant. We accept the following indexing of these axes (fig.1,2). For such indexing stochastic matrices of the Markovian process, giving magnetic moment motion, look in a following way

$$P^{(6)} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & \bar{1} & \bar{2} & \bar{3} \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ \bar{1} \\ \bar{2} \\ \bar{3} \end{matrix} & \begin{pmatrix} -4p-q & p & p & q & p & p \\ p & -4p-q & p & p & q & p \\ p & p & -4p-q & p & p & q \\ q & p & p & -4p-q & p & p \\ p & q & p & p & -4p-q & p \\ p & p & q & p & p & -4p-q \end{pmatrix} \end{matrix},$$

$$P^{(8)} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & \bar{1} & \bar{2} & \bar{3} & \bar{4} \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ \bar{1} \\ \bar{2} \\ \bar{3} \\ \bar{4} \end{matrix} & \begin{pmatrix} s & p & q & p & r & q & p & q \\ p & s & p & q & q & r & q & r \\ q & p & s & p & p & q & r & q \\ p & q & p & s & q & p & q & r \\ r & q & p & q & s & p & q & p \\ q & r & q & p & p & s & p & q \\ p & q & r & q & q & p & s & p \\ q & p & q & r & p & q & p & s \end{pmatrix} \end{matrix},$$

$$s = -3p - 3q - r.$$

Spectral analysis of such matrices is well known [2],[9],[10]. In particular  $P^{(8)}$  has two single eigenvalues and two triple ones ( $\rho = \lambda_1 = 0$ ,  $\eta = \lambda_2 = \lambda_3 = \lambda_4 = -2(p+2q+r)$ ,  $\xi = \lambda_5 = \lambda_6 = \lambda_7 = -4(p+q)$ ,  $\zeta = \lambda_8 = -(6p+4q)$ ), and  $P^{(6)}$  has one single, one double and one triple eigenvalues ( $\rho = \lambda_1 = 0$ ,  $\zeta = \lambda_2 = \lambda_3 = -6p$ ,  $\xi = \lambda_4 = \lambda_5 = \lambda_6 = -4p-2q$ ). In connection with degeneration there is some arbitrariness in choice of eigenvalues, which can be eliminated by the requirement of definite symmetry of eigenvectors with respect to turns around quantization axis  $z$  (quantization axis direction for 3-axial case is different from [2] and this is connected with natural for giving case symmetry). In the case of  $N = 8(6)$  in the capacity of such eigenvectors let us choose states, that under turning at angle  $\frac{\pi}{2}(\frac{2\pi}{3})$  around quantization axis  $z$  obtain factor  $c_n = i^n$ ,  $n = 0, 1, 2, 3 (= \exp(\frac{2\pi i n}{3}), n = 0, 1, 2)$ . In the case of  $N = 8$  such vectors are the following

$$K_n = \frac{1}{4} [|1\rangle + c_n|2\rangle + c_n^2|3\rangle + c_n^3|4\rangle + |\bar{1}\rangle + c_n|\bar{2}\rangle + c_n^2|\bar{3}\rangle + c_n^3|\bar{4}\rangle],$$

$$\tilde{K}_n = \frac{1}{4} [|1\rangle + c_n|2\rangle + c_n^2|3\rangle + c_n^3|4\rangle - |\bar{1}\rangle - c_n|\bar{2}\rangle - c_n^2|\bar{3}\rangle - c_n^3|\bar{4}\rangle],$$

and in the case  $N = 6$

$$K_n = \frac{1}{\sqrt{12}} [|1\rangle + c_n|2\rangle + c_n^2|3\rangle + |\bar{1}\rangle + c_n|\bar{2}\rangle + c_n^2|\bar{3}\rangle],$$

$$\tilde{K}_n = \frac{1}{\sqrt{12}} [|1\rangle + c_n|2\rangle + c_n^2|3\rangle - |\bar{1}\rangle - c_n|\bar{2}\rangle - c_n^2|\bar{3}\rangle].$$

In this connection matrix  $P^{(8)}$  is diagonal in basis  $(K_0, K_1, K_2, K_3, \tilde{K}_0, \tilde{K}_1, \tilde{K}_2, \tilde{K}_3)$  and takes form

$$P^{(8)} = \frac{1}{2} \text{diag}(\rho, \xi, \xi, \xi, \eta, \eta, \zeta, \eta),$$

and matrix

$$P^{(6)} = \frac{1}{2} \text{diag}(\rho, \zeta, \zeta, \xi, \xi, \zeta)$$

in basis  $(K_0, K_1, K_2, \tilde{K}_0, \tilde{K}_1, \tilde{K}_2, )$ .

It should be noted, that strictly speaking the use of probability transition matrices in produced form is certain assumption, i.e., is adjustment to real continuous diffusion process. However, in the case of small diffusion (or, that is the same, diffusion at strong fields) these matrices one can get directly from continuous diffusion model [3],[4] on the base of strict asymptotic analysis of the diffusion operator. In addition it is found that nonzero transition probabilities are only those, that correspond to transition between potential wells, having attraction domains with common boundary. For matrix  $P^{(8)}$  this means that  $q = r = 0$ , and for  $P^{(6)}$  that  $q = 0$ . Moreover, calculations show that one can obtain symmetrical Markovian matrices only for the case of potential drift field. Non-symmetrical field automatically means that transition probability from one easy magnetization direction to another is not equal to the inverse one.

### 3 Reduction of Superoperator $\hat{G}^{-1}$ to Block Form

Since superoperator  $\hat{G}$  is invariant with respect to group  $C_4(C_3)$  action, it is necessary to study transformations properties of complete space of quantum-stochastic states respectively on such action, i.e., to construct basic elements of complete space of states, that under turning of coordinate system on angle  $\frac{\pi}{2}(\frac{2\pi}{3})$  obtain factor  $c_n$ . According to selection rules [8] superoperator  $\hat{G}$  in such basis is of block structure. For this aim it is naturally in quantum variables space to extract states with such properties relatively group  $C_4(C_3)$  (such kind of states in stochastic variables space we have constructed above) and than to construct 4(3) nonoverlapping subspaces of complete quantum-stochastic space, the states of which obtain factor  $c_n$  under turning at angle  $\frac{\pi}{2}(\frac{2\pi}{3})$  around quantization axis  $z$ . How it is shown in [2], invariant with respect to group  $C_4$  subspace in the case  $N = 8$  is divided into two nonoverlapping subspaces with different properties relatively time inversion (symmetry and asymmetry subspaces). Really, all others subspaces also suppose such division both in 4- and 3-axial cases and also at other symmetries under proper disposition (consistent with the symmetry) of coordinate system. So it is possible to construct basis in which superoperator  $\hat{G}$  consists of 8(6) equal blocks of order  $8 \times 8$ , that differ from each other only by diagonal elements, composed of stochastic matrix eigenvalues combinations. Nondiagonal part of each block is determined only by the transition structure

of nuclear system and does not depend on sign of magnetic anisotropy constant. Denoting by  $\{n\pm\}$  blocks  $\begin{pmatrix} \text{symmetrical} \\ \text{asymmetric} \end{pmatrix}$  with respect to time reversal, that obtain factor  $c_n = i^n$ ,  $n = 0, 1, 2, 3$  ( $\exp(\frac{2\pi i n}{3})$ ),  $n = 0, 1, 2$ ) for 4(3)-axial case and denoting quantum transition operators

$$\alpha = |\frac{1}{2}\rangle\langle\frac{1}{2}|, \beta = |\frac{-1}{2}\rangle\langle\frac{-1}{2}|, \gamma = |\frac{3}{2}\rangle\langle\frac{1}{2}|, \sigma = |\frac{-3}{2}\rangle\langle\frac{-1}{2}|,$$

$$\delta = |\frac{1}{2}\rangle\langle\frac{-1}{2}|, \varepsilon = |\frac{-1}{2}\rangle\langle\frac{1}{2}|, \mu = |\frac{3}{2}\rangle\langle\frac{-1}{2}|, \nu = |\frac{-3}{2}\rangle\langle\frac{1}{2}|,$$

we have the following basic functions for blocks  $\{n\pm\}$  in 4-axial case

$$|1\rangle = K_n(\alpha \mp \beta), |2\rangle = K_{n+3}\delta \pm K_{n+1}\varepsilon, |3\rangle = K_{n+3}\gamma \pm K_{n+1}\sigma,$$

$$|4\rangle = K_{n+2}(\mu \mp \nu), |5\rangle = \bar{K}_{n+2}(\mu \pm \nu), |6\rangle = \bar{K}_{n+3}\gamma \mp \bar{K}_{n+1}\sigma,$$

$$|7\rangle = \bar{K}_{n+3}\delta \mp \bar{K}_{n+1}\varepsilon, |8\rangle = \bar{K}_n(\alpha \pm \beta),$$

and in 3-axial case

$$|1\rangle = K_n(\alpha \mp \beta), |2\rangle = K_{n+2}\delta \pm K_{n+1}\varepsilon, |3\rangle = K_{n+2}\gamma \pm K_{n+1}\sigma,$$

$$|4\rangle = K_{n+1}\mu \mp K_{n+2}\nu, |5\rangle = \bar{K}_{n+1}\mu \pm K_{n+2}\nu, |6\rangle = \bar{K}_{n+2}\gamma \mp \bar{K}_{n+1}\sigma,$$

$$|7\rangle = \bar{K}_{n+2}\delta \mp \bar{K}_{n+1}\varepsilon, |8\rangle = \bar{K}_n(\alpha \pm \beta),$$

Here in the 4(3)-axial cases all indexes are taken by  $\text{mod}4(3)$ . In this basis diagonal submatrix  $P_{n\pm}$  takes form for 4-axial case

$$P_{0\pm} = -\text{diag}(\Lambda, \Omega, \Omega, \Omega, \Xi, \Upsilon, \Upsilon, \Upsilon) \quad (7)$$

$$P_{1,3\pm} = -\text{diag}(\Omega, \frac{\Omega}{2}, \frac{\Omega}{2}, \frac{\Omega}{2}, \Upsilon, \Theta, \Theta, \Upsilon)$$

$$P_{2\pm} = -\text{diag}(\Omega, \Omega, \Omega, \Lambda, \Upsilon, \Upsilon, \Upsilon, \Xi),$$

where  $\Lambda = 0$ ,  $\Omega = 4p + 4q$ ,  $\Xi = 6p + 2r$ ,  $\Upsilon = 2p + 4q + 2r$ ,  $\Theta = 4p + 2q + 2r$ . For  $N = 6$  we have

$$P_{0\pm} = -\text{diag}(\Lambda, \Omega, \Omega, \Omega, \Upsilon, \Upsilon, \Upsilon, \Upsilon), \quad (8)$$

$$P_{1,2\pm} = -\text{diag}(\Omega, \frac{\Omega}{2}, \frac{\Omega}{2}, \frac{\Omega}{2}, \Upsilon, \Upsilon, \Upsilon, \Upsilon),$$

where  $\Lambda = 0$ ,  $\Omega = 6p$ ,  $\Upsilon = 4p + 2q$ .

Superoperator  $\hat{L}$  action at all received subspaces independently on symmetry appears to be the same and is given by matrix

$$\hat{L} = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix},$$

$$D = \begin{pmatrix} 0 & A^e/\sqrt{2} & (2A^e - A^g)/\sqrt{6} & (A^e - A^g)/2\sqrt{3} \\ A^e/\sqrt{2} & 0 & (A^e + A^g)/2\sqrt{3} & -(A^g + 2A^e)/\sqrt{6} \\ -A^g/\sqrt{6} & (3A^e - A^g)/2\sqrt{3} & 0 & A^e/\sqrt{2} \\ (3A^e + A^g)/2\sqrt{3} & -A^g/\sqrt{6} & A^e/\sqrt{2} & 0 \end{pmatrix}.$$

Block of form  $D$  was introduced first in [2] for invariant subspace of quantum-stochastic states antisymmetrical with respect to time inversion (we denote this subspace as 0-) in the case  $N = 8$ . Remarkably, that other blocks of superoperator  $\hat{L}$  (that have another symmetry, i.e., that obtain factor  $c_n$  under turning of coordinate system on angle  $\frac{\pi}{2}(\frac{2\pi}{3})$ ) have the same form. Moreover, one can show that the same form of elementary block remains for certain other symmetries, for example for tetrahedron symmetry, cylindrical symmetry and some others. So elementary block  $D$  is in some sense universal.

## 4 Spectral Analysis of Quantum-Stochastic Superoperator

Last paragraph is devoted to reduction of quantum-stochastic superoperator to block-diagonal form convenient for calculations its spectral characteristics (eigenvalues and eigenvectors). This problem can be solved under assumption that one of terms  $\hat{L}$  or  $\hat{P}$  composite superoperator  $\hat{G}^{-1}$  is small in comparison with another. It is naturally to assume smallness of stochastic term  $\hat{P}$ . Note that eigenvalues of unperturbed superoperator  $\hat{L}$  are known explicitly. These eigenvalues are the super-fine transition frequencies  $\lambda_{\pm i} = \pm b_i$ , where  $b_1 = \frac{1}{2}(3A^e - A^g)$ ,  $b_2 = \frac{1}{2}(A^e - A^g)$ ,  $b_3 = -\frac{1}{2}(A^e + A^g)$ ,  $b_4 = -\frac{1}{2}(3A^e + A^g)$ . Corresponding eigenfunctions have the form [2]

$$\begin{aligned} \Psi_{\pm 1} &= \frac{1}{2}|1\rangle + 0 + \frac{1}{\sqrt{6}}|3\rangle + \frac{1}{2\sqrt{3}}|4\rangle \pm \left(\frac{1}{6}|5\rangle + \frac{\sqrt{2}}{3}|6\rangle + \frac{1}{\sqrt{6}}|7\rangle + \frac{1}{2\sqrt{3}}|8\rangle\right) \\ \Psi_{\pm 2} &= \frac{1}{\sqrt{6}}|1\rangle - \frac{1}{2\sqrt{3}}|2\rangle - \frac{1}{\sqrt{3}}|3\rangle + 0 \pm \left(-\frac{1}{\sqrt{6}}|5\rangle - \frac{1}{2\sqrt{3}}|6\rangle + \frac{1}{2}|7\rangle + 0\right) \\ \Psi_{\pm 3} &= \frac{1}{2\sqrt{3}}|1\rangle + \frac{1}{\sqrt{6}}|2\rangle + 0 - \frac{1}{2}|4\rangle \pm \left(\frac{1}{2\sqrt{5}}|5\rangle - \frac{1}{\sqrt{6}}|6\rangle + 0 + \frac{1}{2}|8\rangle\right) \end{aligned}$$



$$\Psi_{\pm 4} = 0 - \frac{1}{2}|2\rangle + \frac{1}{2\sqrt{3}}|3\rangle - \frac{1}{\sqrt{6}}|4\rangle \pm (\frac{\sqrt{2}}{3}|5\rangle - \frac{1}{6}|6\rangle + \frac{1}{2\sqrt{3}}|7\rangle - \frac{1}{\sqrt{6}}|8\rangle).$$

Standard perturbation theory in the case of absence of degeneration let us calculate eigenvalues corrections

$$\Delta\lambda_k = \langle \Psi_k | i\hat{P} | \Psi_k \rangle$$

and also eigenvectors corrections. In our case for eigenvalues this leads to results reduced in Tab.1 of eigenvalues corrections.

**Tab.1a.** *Eigenvalues corrections for 4-axis case.*

	block 0 $\pm$	block 1, 3 $\pm$	block 2 $\pm$
$\delta\lambda_1$	$i(19/9p + 26/9q + r)$	$i(31/9p + 26/9q + r)$	$i(3p + 10/3q + r)$
$\delta\lambda_2$	$i(3p + 8/3q + r)$	$i(3p + 8/3q + r)$	$i(3p + 4q + r)$
$\delta\lambda_3$	$i(3p + 10/3q + r)$	$i(3p + 10/3q + r)$	$i(3p + 2q + r)$
$\delta\lambda_4$	$i(35/9p + 28/9q + r)$	$i(23/9p + 28/9q + r)$	$i(3p + 8/3q + r)$

**Tab.1b.** *Eigenvalues corrections for 3-axis case.*

	block 0 $\pm$	block 1, 2 $\pm$
$\delta\lambda_1$	$i(3, 5p + q)$	$i(4, 25p + q)$
$\delta\lambda_2$	$i(4p + q)$	$i(4p + q)$
$\delta\lambda_3$	$i(4, 5p + q)$	$i(3, 75p + q)$
$\delta\lambda_4$	$i(5p + q)$	$i(3, 5p + q)$

## 5 $J$ -Selfadjointness and Qualitative Spectrum Behavior

Reductions of operator matrix  $\hat{L} + i\hat{P}$  to block-diagonal form at mentioned basis permit to receive effective way of calculating of line shape reduce to inversion of matrices of  $8 \times 8$ -order corresponding to each block. In the case of equilibrium initial distribution resonance absorption spectrum is described by the only block of the superoperator  $\hat{L} + i\hat{P}$ , namely by that, which is invariant with respect to turns on angle  $\frac{\pi}{2}(\frac{2\pi}{3})$  and antisymmetrical relatively time inversion. But if the initial distribution is arbitrary one it is necessary to know all blocks of the superoperator  $\hat{L} + i\hat{P}$  for line shape determination.

The superoperator  $\hat{L} + i\hat{P}$  spectrum is, generally speaking, complex one, nevertheless, it is possible to get qualitative information on spectrum behavior at different relations between parameters of magnetic and electron spin systems. The superoperator  $\hat{L} + i\hat{P}$  spectrum lies at lower half-plane and is placed symmetrically relatively

imaginary axis. This follows from  $J$ -selfadjointness of  $\hat{L} + i\hat{P}$ . Really

$$J\left(\begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix} + i\hat{P}\right)J = \left(\begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix} + i\hat{P}\right)^\dagger,$$

when  $J = \text{diag}(1, 1, 1, 1, -1, -1, -1, -1)$ .

Let us consider for illustration the case of equilibrium initial distribution, which is described by block 0-. At the limit case of fast relaxation (at high temperatures) eigenvalues of this block (just as of any other block) belong to imaginary axis, and this case corresponds to resonance absorption spectrum consisting of the only line of Lorentz width on the frequency  $\omega$ . At diminishing of relaxation eigenvalues as before some time belong to imaginary axis moving on it, because at fast relaxation limit there are two single and two triple eigenvalues both in 4- and 3-axial case (7),(8), but due to the  $J$ -selfadjointness eigenvalues can leave imaginary axis only by pairs. At certain moment one of pairs will diverge (and also this can be not one pair from initially existing pairs in triple eigenvalues but one of anew formed in a process of random walk along imaginary axis). In this connection resonance absorption spectrum will have a form of two lines of certain width, symmetrical relatively frequency  $\omega$ . Under further diminishing of relaxation parameters new pairs of lines appear, and the width is decreased. At limit all eigenvalues of the matrix come down from imaginary axis and are dropped on real axis, that on resonance absorption spectrum correspond to line shape with peaks on frequencies  $\omega + b_{\pm i}$  (frequencies  $b_{\pm 4}$  are prohibited and don't appear on spectrum), the width is decreased as far as eigenvalues approach real axis, i.e., under diminishing of relaxation or, that is the same, of temperature.

It is necessary to note that symmetrical line shape corresponds to potential drift field (in DOM — to symmetrical matrices  $P$ ). Calculations using non-symmetrical transition probabilities demonstrate non-symmetrical line shape with respect to main frequency  $\omega$ .

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**fig. 1. Mutual disposition of the easy magnetization directions and coordinate system (4-axis case, N=8).**

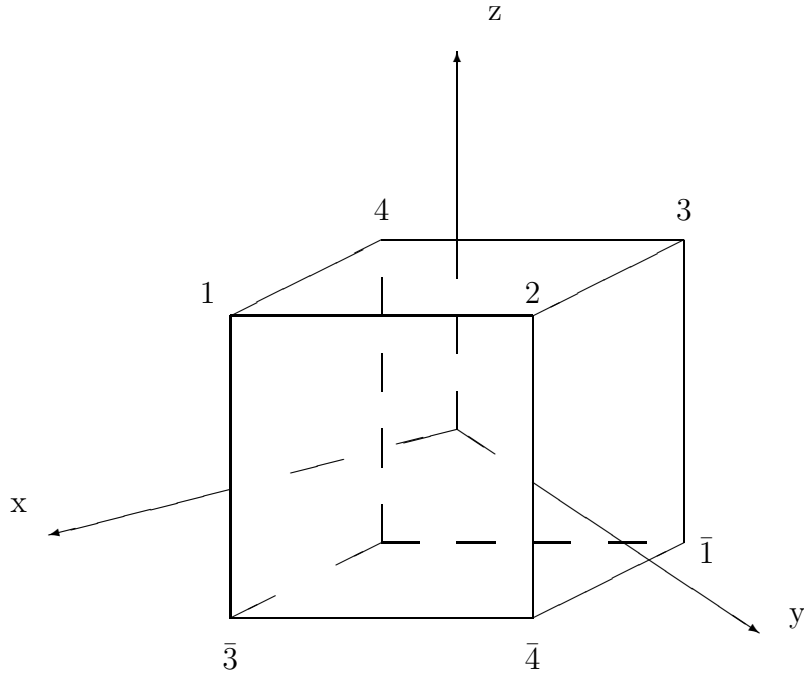
*Values of unit vector  $\vec{m}$  of particle magnetization*

$$\vec{m} = \pm \vec{m}_i, \quad i = 1, 2, 3, 4.$$

$$\vec{m}_1 = (\sqrt{2/3}, 0, 1/\sqrt{3}), \quad \vec{m}_2 = (0, \sqrt{2/3}, 1/\sqrt{3}),$$

$$\vec{m}_3 = (-\sqrt{2/3}, 0, 1/\sqrt{3}), \quad \vec{m}_4 = (0, -\sqrt{2/3}, 1/\sqrt{3}).$$

*Easy magnetization directions coincide with ones from the center of cube to its vertices.*



**fig. 2. Mutual disposition of the easy magnetization directions and coordinate system (3-axis case, N=6).**

*Values of unit vector  $\vec{m}$  of particle magnetization*

$$\vec{m} = \pm \vec{m}_i, \quad i = 1, 2, 3.$$

$$\vec{m}_1 = (\sqrt{\frac{2}{3}}, 0, \frac{1}{\sqrt{3}}), \quad \vec{m}_2 = (\frac{-1}{\sqrt{6}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}), \quad \vec{m}_3 = (\frac{-1}{\sqrt{6}}, \frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{3}}).$$

*Easy magnetization directions coincide with ones from the center of cube to the centers of its faces.*

